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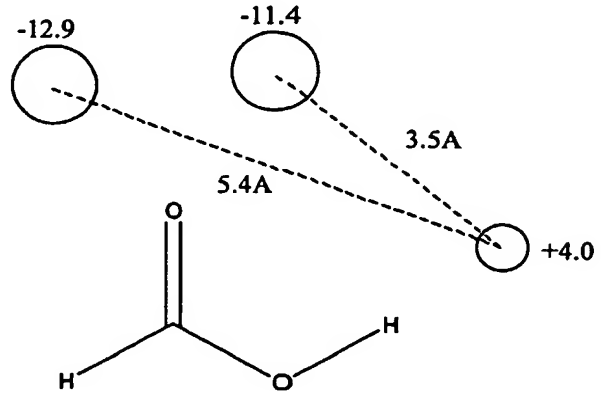
(54) Title: COMPARISON OF MOLECULES USING FIELD POINTS



(57) Abstract: A method of comparing two conformers in which an overlay score is obtained by determining the field value for molecule A at the coordinates of molecule B's field point. Molecule B's field point does not have to be very close to molecule A's field point to get a good overlay score: it just needs to be in a region where molecule A's field is large. This overcomes a limitation of conventional pseudo-Coulombic scoring in which a low score is achieved when extrema of large extent overlap but have their minimum points widely separated. The method can be applied to molecular mechanics modelling using atom centred charges (ACCs) and extended electron distributions (XEDs) as well as to quantum mechanics models.

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